FMOCS IV @ PoCheMoN 2016

Joint Meeting

Frontiers in Metal-Oxide Cluster Science IV
and
Final Meeting of COST Action CM1203
Polyoxometalate Chemistry for Molecular Nanoscience 2016

Programme and Abstracts

10 - 14 July 2016
Newcastle University
Newcastle upon Tyne, UK

cost
EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

Detailed Conference Programme

Sunday 10th July

11:00 – 13:00		Registration
13:00 – 13:30		Opening Remarks

Session Chair **R. J. Errington**

13:30 – 14:00	**K01**	Marcella **Bonchio**, *University of Padova* Bio-inspired Nano-architectures for Artificial Photosynthesis
14:00 – 14:30	**K02**	Josep M. **Poblet,** *URV Tarragona* Catalytic reactions involving functionalized polyoxometalates
14:30 – 14:45	**C01**	Laurent **Ruhlmann,** *Université de Strasbourg* Porphyrin-Polyoxometalate Electropolymers for the Photoelectrochemical Energy Conversion
14:45 – 15:00	**C02**	Soumyabrata **Roy,** *Jawaharlal Nehru Centre for Advanced Scientific Research* Decavanadate Based Hetero-metallic Inorganic-organic Hybrids as Highly Active Electro-catalysts for Hydrogen Evolution
15:00 – 15:30	**K03**	Yang-Guang **Li,** *Northeast Normal University* Polyoxometalate-originated high efficient non-noble-metal electrocatalysts for hydrogen evolution reaction
15:30 – 16:00		Coffee Break

Session Chair **J.-M. Poblet**

16:00 – 16:30	**K04**	Carles **Bo,** *ICIQ Tarragona* Exploring the PoCheMoN World with “in-silico” tools
16:30 – 17:00	**K05**	Colette **Boskovic,** *University of Melbourne* Lanthanoid-Polyoxometalates: Single-Molecule Magnetism, Inelastic Neutron Scattering and Ab Initio Studies
17:00 – 17:15	**C03**	Beñat **Artetxe,** *Universidad del País Vasco* New Perspectives for Old Clusters: Anderson–Evans Anions as Building Blocks of Heterometallic 3d–4f POM Frameworks
17:15 – 17:30	**C04**	Bassem S. **Bassil,** *Jacobs University* Lacunary Heteropolytungstates Stabilizing Polynuclear Magnetic 3d-Transition Metal Cores
17:30 – 18:00	**K06**	Emmanuel **Cadot,** *Institut Lavoisier, Université Versailles* About Supramolecular Chemistry with Very Large Polyoxometalates
18:00 – 18:30	**K07**	Helena I. S. **Nogueira,** *University of Aveiro* Raman imaging and SERS studies on polyoxometalates and its nanocomposites

Monday 11th July

Session Chair **M. Bonchio**

9:00 – 9:30	**K08**	Craig L. **Hill,** *Emory University* Counter Cation Studies in New POM-based Materials
9:30 – 9:45	**C05**	Pawel J. **Kulesza,** *University of Warsaw* Importance of Specific Metal-Polyoxometallate Interactions in Efficient Charge Propagation and Electro(photo)catalysis
9:45 – 10:00	**C06**	Roy E. **Schreiber,** *Weizmann Institute of Science* Colloids of POMs as a Mechanistic Step for Chemical Reactivity
10:00 – 10:30	**K09**	Sayaka **Uchida,** *The University of Tokyo* Reduction-Induced Uptake of Alkali Metal Cations by Porous Ionic Crystals based on Polyoxomolybdates
10:30 – 11:00		Coffee Break

Session Chair **E. Cadot**

11:00 – 11:30	**K10**	Ulrich **Kortz,** *Jacobs University* Recent Developments in Polyoxopalladate Chemistry
11:30 – 11:45	**C07**	Feng **Xu,** *Hunan University* Complex Assembly of {Cu_6}-Incorporated Icosametallic Clusters
11:45 – 12:00	**C08**	Anne-Lucie **Teillout,** *Université Paris-Sud* The Wells-Dawson Polyoxotungstates: re-exploring their electrochemical behaviour in solution
12:00 – 12:30	**K11**	Maxim N. **Sokolov,** *Nikolaev Institute of Inorganic Chemistry* New polyoxometalate complexes of noble metals
12:30 – 13:30		Lunch Break

Session Chair **A. Proust**

13:30 – 14:00	**K12**	R. John **Errington,** *Newcastle University* New Insight, Further Questions: Targeted Non-Aqueous Polyoxometalate Synthesis
14:00 – 14:30	**K13**	Yongge **Wei,** *Tsinghua University* Chemical Modification of Polyoxometalates and their Applications
14:30 – 14:45	**C09**	Wassim **Ayass,** *Jacobs University* Introducing Thallium in Polyoxometalate Chemistry
14:45 – 15:00	**C10**	Natalya V. **Izarova,** *Peter Grünberg Institute* Palladate/Tungstate Hybrids
15:00 – 15:30	**K14**	Chris **Ritchie,** *University of Melbourne* Microwave assisted synthesis, structural isomers and more…
15:30 – 16:00		Coffee Break

Session Chair **Y.-G. Li**

16:00 – 16:30	**K15**	Ronny **Neumann,** *Weizmann Institute* The Importance of Electron Transfer in Polyoxometalate-Catalysed Reactions: Photoelectrochemical Reduction of CO_2 and Electron-Transfer Oxidation of Benzene
16:30 – 17:00	**K16**	Oxana A. **Kholdeeva,** *Boreskov Institute of Catalysis* Aromatic oxidations with di-vanadium-substituted γ-Keggin polyoxotungstate: new reactions, mechanistic insights and immobilization approaches
17:00 – 17:15	**C11**	De-Liang **Long,** *University of Glasgow* Constructing high nuclearity polyoxotungstates with the aid of silver(I) counter-cation
17:15 – 17:30	**C12**	Nataliya V. **Maksimchuk,** *Boreskov Institute of Catalysis* Mono- and di-titanium-substituted Lindqvist tungstates as catalysts for heterolytic activation of H_2O_2
17:30 – 18:00	**K17**	Pierre **Mialane,** *Université de Versailles* Using the Robustness of Polyoxometalates for the Elaboration of Materials with Properties Ranging from Magnetic to Optical
18:00 – 18:30	**K18**	Ryo **Tsunashima** , *Yamaguchi University* Mixed-valence Polyoxometalate; a molecular nanoparticle for macroscopic electrical properties

Tuesday, 12th July

Session Chair **L. Cronin**

9:00 – 9:30	**K19**	Tatjana N. **Parac-Vogt,** *KU Leuven* Metal-substituted polyoxometallates as artificial nucleases
9:30 – 9:45	**C13**	Jorge J. **Carbó,** *Universitat Rovira i Virgili, Tarragona* Computational modeling of polyoxometalate-protein interactions

9:45 – 10:00	**C14**	Thi Kim Nga **Luong,** *KU Leuven* Detailed Mechanism of ATP Hydrolysis Promoted by a Binuclear Zr^{IV}-Substituted Keggin Polyoxometalate Elucidated by a Combination of ^{31}P, ^{31}P DOSY and ^{31}P EXSY NMR Spectroscopy
10:00 – 10:30	**K20**	Lixin **Wu,** *Jilin University* Induced Chirality and Chirality Transfer in Polyoxometalate Systems
10:30 – 11:00		Coffee Break

Session Chair L. Wu

11:00 – 11:30	**K21**	Lee **Cronin,** *University of Glasgow* Mechanism of Self Assembly of Gigantic Inorganic Clusters
11:30 – 11:45	**C15**	Nuno A. G. **Bandeira,** *ICIQ, Barcelona Institute of Science and Technology* Structural Changes of a Vanadium Polyoxoanion: A Mystery
11:45 – 12:00	**C16**	Santiago **Reinoso,** *Universidad del País Vasco* Thermo-Structural Studies in Vanadate–Metalorganic Hybrid Compounds: Dynamic vs. Robust Open-Framework Materials
12:00 – 12:30	**K22**	Yu-Fei **Song,** *Beijing University of Chemical Technology* Polyoxometalate-functionalized nanocarbon as energy materials
12:30 – 13:30		Lunch Break

Session Chair U. Kortz

13:30 – 14:00	**K23**	Eugenio **Coronado,** *ICMol, University of Valencia* Magnetic polyoxometalates for quantum technologies
14:00 – 14:30	**K24**	John **Fielden,** *University of East Anglia* Donor-Acceptor Organo-Imido POMs: New Materials for Photonics and Solar Energy Conversion
14:30 – 14:45	**C17**	Qi **Zheng,** *University of Glasgow* Following the Reaction of Heteroanions inside a $\{W_{18}O_{56}\}$ Polyoxometalate Nanocage by NMR Spectroscopy and Mass Spectrometry
14:45 – 15:00	**C18**	Jingli **Xie,** *Jiaxing University* STM Investigation of the Co-assembly Behaviour of POMs clusters with Host Molecule 1,3,5-tris(10-carboxydecyloxy)benzene (TCDB)
15:00 – 15:30	**K25**	Dominique **Vuillaume,** *CNRS, Lille* Optical and electrical properties of molecular junctions and networks
15:30 – 16:00		Coffee Break

Session Chair I. Weinstock

16:00 – 16:30	**K26**	Walter G. **Klemperer,** *University of Illinois* Why Do Highly-Charged Polyions with Univalent Counterions Form Spherical Shells – an Unanswered Question?
16:30 – 17:00	**K27**	Sebastian **Polarz,** *University of Konstanz* Organic-Inorganic Surfactants: Hybrids with Polyoxometalate Heads and Beyond
17:00 – 17:15	**C19**	Pavel A. **Abramov,** *Nikolaev Institute of Inorganic Chemistry* From giant chalcoPOMs to giant polyoxoniobates
17:15 – 17:30	**C20**	Zhengguo **Lin,** *Jacobs University* Chiral Dodecanuclear Palladium(II)-Thio Cluster: Synthesis, Structure, and Formation Mechanism
17:30 – 18:00	**K28**	Haralampos N. **Miras,** *University of Glasgow* Directed Self-Assembly, Electronic Modulation and Isomer “locking” in POM systems
18:00 – 18:30	**K29**	Paul **Kögerler,** *RWTH Aachen* Revisiting some polyoxometalate archetypes

Detailed Mechanism of ATP Hydrolysis Promoted by a Binuclear Zr^{IV}-Substituted Keggin Polyoxometalate Elucidated by a Combination of ^{31}P, ^{31}P DOSY and ^{31}P EXSY NMR Spectroscopy

Thi Kim Nga Luong,[1,*] *Pavletta Shestakova*,[1,2] *Gregory Absillis*,[1] and *Tatjana N. Parac-Vogt* [1]

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[2] NMR Laboratory, Institute of Organic Chemistry with Centre of Phytochemistry Bulgarian Academy of Sciences, Bulgaria

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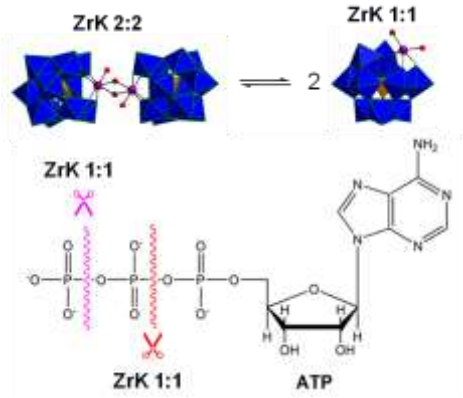
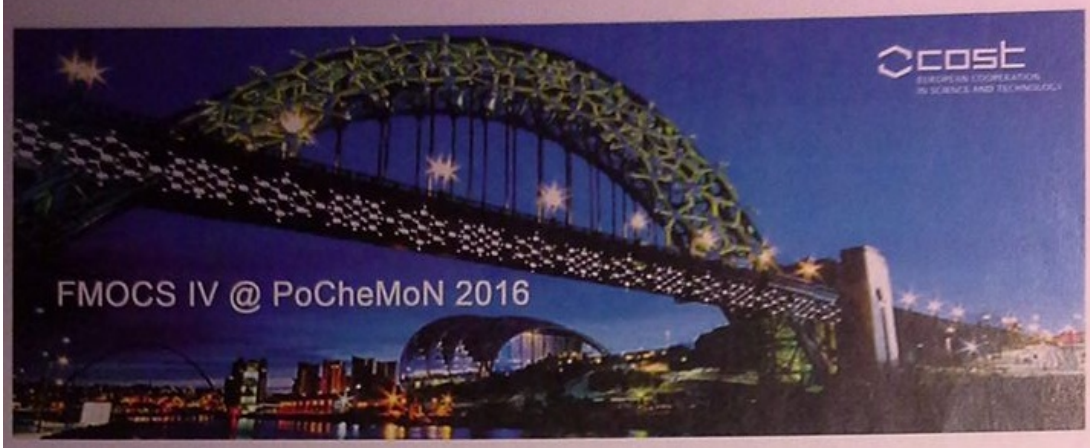
The full reaction mechanism of adenosine triphosphate (ATP) hydrolysis in the presence of the binuclear Zr^{IV}-substituted Keggin type polyoxometalate $(Et_2NH_2)_8[\{\alpha\text{-}PW_{11}O_{39}Zr(\mu\text{-}OH)(H_2O)\}_2]\cdot 7H_2O$ (ZrK 2:2) at pD 6.4 and 50 °C was elucidated by a combination of ^{31}P, ^{31}P DOSY and ^{31}P EXSY NMR spectroscopy, demonstrating the potential of these techniques for the analysis of complex reaction mixtures involving polyoxometalates (POMs). ^{31}P and ^{31}P DOSY NMR measured for pure ZrK 2:2 and for the solution containing ZrK 2:2 and ATP at pD 6.4 shows that in the presence of ATP, ZrK 2:2 converts into the more active species ZrK 1:1 and this species is responsible for the hydrolysis of the phosphoanhydride bonds.[1] Two possible parallel reaction pathways were proposed on the basis of the observed reaction intermediates and final products. The ^{31}P spectrum of a mixture of 20.0 mM ATP and 3.0 mM ZrK 2:2 at pD 6.4 measured immediately after sample preparation, shows the formation of a complex I1A and I1B between ATP and POM. During the course of the hydrolytic reaction at pD 6.4 and 50 °C, various products including adenosine diphosphate (ADP), adenosine monophosphate (AMP), pyrophosphate (PP) and phosphate (P) were detected. In addition, several intermediate species representing ADP/ZrK 1:1 (I2), AMP/ZrK 1:1 (I3), P/ZrK 1:1 (I4) and PP/ZrK 1:1 (I5) complexes were also identified. ^{31}P EXSY NMR spectra evidenced slow exchange between ATP and I1A, ADP and I2, and PP and I5.



1. T. K. N. Luong, P. Shestakova , T. T. Mihaylov, G. Absillis, K. Pierloot and T. N. Parac-Vogt, *Chemistry – A European Journal*, 2015, **21**, 4428-4439.



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Certificate of Attendance

This is to certify that Thi Kim Nga **Luong**

has participated in the joint meeting involving the fourth *Frontiers in Molecular Oxide Cluster Science* symposium and the final conference of COST Action CM1203, PoCheMoN 2016 held at Newcastle University from 10th to 14th July 2016.

Newcastle upon Tyne, July 14th 2016

On behalf of the Organising Committee

R. J. Errington

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